Topics for Quiz 4 Nov. 19ths 2011 Chenguang Ji

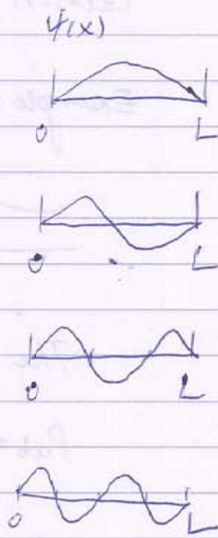
— De Broglie waves
— Schrödinger equation, Born interpretation of wavefunction
  Stationary / non-stationary solution
— Expectation, uncertainty of physical quantities for a given state
  Heisenberg uncertainty principle

I De Broglie waves

A particle of matter with momentum p could act as a wave with wavelength:

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$$, smaller $m \Rightarrow$ longer $\lambda \Rightarrow$ stronger interference / diffraction effects

Example 1: a particle in a box:



Solution: quantized wavelength:

$$n \cdot \lambda_n = 2L$$

$$\Rightarrow \lambda_n = \frac{2L}{n}$$

De Broglie relation:

$$p_n = \frac{h}{\lambda_n} = \cancel{\frac{h}{(n/2L)}} = \frac{h}{(2L/n)}$$

$$= \frac{2\pi\hbar}{2L} \cdot n = \frac{\pi\hbar}{L} \cdot n$$

Kinetic energy $= \frac{p_n^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{\pi n}{L}\right)^2$.

Consistent with the solution of Schrödinger equation.

II Schrödinger equation:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H}\Psi(x,t) \quad (\text{time-dependent S.E.})$$

where,

$\Psi(x,t)$ is the wavefunction of a particle experiencing a given potential $V(x)$;

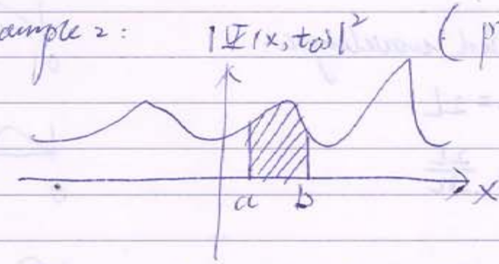
All the physical information of the particle can be extracted from $\Psi(x,t)$;

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m}}_{\text{K.E.}} + \underbrace{\hat{V}}_{\text{P.E.}}$$

Born interpretation:

$|\Psi(x,t)|^2$: probability density

Example 2: $|\Psi(x,t_0)|^2$ (probability density at a given time t_0)



The probability to detect the particle within $[a,b]$ is

$$P_{ab} = \int_a^b |\Psi(x,t_0)|^2 dx$$

This naturally leads to the normalization condition:

$$\lim_{\substack{b\to+\infty \\ a\to-\infty}} \int_a^b |\Psi(x,t_0)|^2 dx = \int_{-\infty}^{+\infty} |\Psi(x,t_0)|^2 dx \equiv 1$$

Stationary solutions:

a set of specific solutions to S.E. with the form of:

$$\Psi(x,t) = \underbrace{\psi(x)}_{\text{only depends on spatial coordinates}} \underbrace{e^{-\frac{iEt}{\hbar}}}_{\text{only depends on time}} = \psi(x)\, e^{-i\omega t}, \text{ where } \omega = \frac{E}{\hbar}$$

where,

$$(\underbrace{\frac{\hat{p}^2}{2m}}_{K.E.} + \underbrace{\hat{V}}_{P.E.})\,\psi(x) = E\,\psi(x) \quad \text{(time-independent S.E.) (TISE)}$$

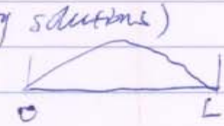
Only some E_s can give solutions to the S.E.. This is usually determined by the boundary conditions.

properties of stationary solutions:

1. probability density is stationary;
2. expectations of physical quantities are stationary.

Example 3: a particle in the box (stationary solutions)

$$\Psi_1(x,t) = \psi_1(x)\, e^{-\frac{iE_1 t}{\hbar}}, \quad \psi_1(x):$$



$$\Psi_2(x,t) = \psi_2(x)\, e^{-\frac{iE_2 t}{\hbar}}, \quad \psi_2(x):$$

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probability density:

$$|\Psi_1(x,t)|^2 = |\psi_1(x)\, e^{-\frac{iE_1 t}{\hbar}}|^2 = |\psi_1(x)|^2: \text{ no time-dependence}$$

similar for $|\Psi_2(x,t)|^2 = |\psi_2(x)|^2$.

expectation

$$\langle \hat{x} \rangle_{\text{state }1}(t) = \int_{-\infty}^{+\infty} \Psi_1^*(x,t) \times \Psi_1(x,t)\, dx$$

$$= \int_{-\infty}^{+\infty} (\psi_1(x) e^{\frac{iE_1 t}{\hbar}})^* \, x \, (\psi_1(x) e^{-\frac{iE_1 t}{\hbar}})\, dx$$

$$= \underline{\int_{-\infty}^{+\infty} \psi_1^*(x)\, x\, \psi_1(x)\, dx}$$

↓ no time-dependence

$$\equiv \frac{L}{2}$$

Question: is the particle moving or not?

Yes. $\Delta p \Delta x \geq \frac{\hbar}{2}$, $\Delta p > 0 \Rightarrow$ finite momentum

$\Rightarrow$ finite velocity

But the expectation of momentum:

$\langle p \rangle$ is stationary, that is, without time-dependence.

Non- stationary solutions (general solutions)

$$\Psi(x,t) = \sum_{n=0,1,2,\cdots} \underbrace{C_n\left[\psi_n(x) e^{-\frac{iE_n t}{\hbar}}\right]}_{\text{stationary solution}}$$

with

normalization condition $\begin{cases} \int_{-\infty}^{+\infty} |\psi_n(x)|^2 dx \equiv 1, \\ \sum_{n=0,1,2,\cdots} |C_n|^2 \equiv 1 \end{cases}$

orthogonality condition:

$$\int_{-\infty}^{+\infty} \psi_n^*(x)\, \psi_m(x)\, dx \equiv 0 \quad \text{for } n \neq m$$

properties of non- stationary solutions :

① probability density has time - dependence ;

② expectations of physical quantities have time- dependence ;

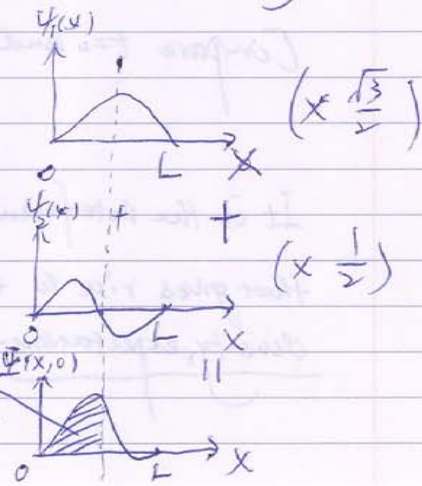
Example 4: particle in a box (non- stationary solutions)

$$\Psi(x,t) = \frac{\sqrt{3}}{2}\left(\psi_1(x) e^{-\frac{iE_1 t}{\hbar}}\right) + \frac{1}{2}\left(\psi_2(x) e^{-\frac{iE_2 t}{\hbar}}\right)$$

probability density:

① at time $t=0$:

$$\Psi(x,0) = \frac{\sqrt{3}}{2}\psi_1(x) + \frac{1}{2}\psi_2(x):$$



The particle is more possible to be ~~fond~~ found in the left half of the box.

② at $t = \dfrac{\pi}{\frac{(E_2 - E_1)}{\hbar}}$

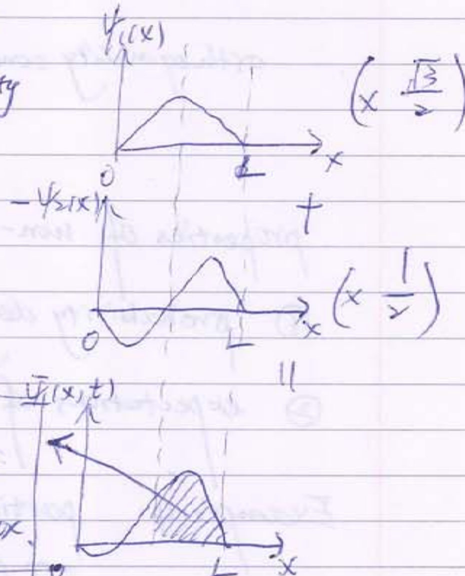
$$\Psi(x,t) = \frac{\sqrt{3}}{2}\psi_1(x) e^{-\frac{iE_1 t}{\hbar}} + \frac{1}{2}\,[\psi_2(x)]\, e^{-\frac{iE_2 t}{\hbar}}$$

$$= e^{-\frac{iE_1 t}{\hbar}}\left[\frac{\sqrt{3}}{2}\psi_1(x) + \frac{1}{2}\psi_2(x) \boxed{e^{\frac{-i(E_2-E_1)t}{\hbar}}}\right]$$

phase difference

$$= \boxed{e^{-\frac{iE_1 t}{\hbar}}}\left[\frac{\sqrt{3}}{2}\psi_1(x) \boxed{-} \frac{1}{2}\psi_2(x)\right]$$

Such a factor does not influence the probability density



Now the particle is more possible to be found in the right half of the box.

Compare $t=0$ and $t = \dfrac{\pi}{\frac{(E_2 - E_1)}{\hbar}} \Rightarrow \langle \hat{x} \rangle$ is time-dependent.

non-stationary.

It is the interference between different stationary-solutions that gives rise to the time-dependence of probability density, expectations. → non-stationary

III expectation, uncertainties:

position: $\hat{x}$, momentum: $\hat{p}$, kinetic energy $\hat{E} = \frac{\hat{p}^2}{2m}$

expectation: $\langle \hat{x} \rangle = \int_{-\infty}^{+\infty} \underbrace{\Psi^*(x,t)\, x\, \Psi(x,t)}_{\hat{x}}\, dx$, $\langle \hat{p} \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t) \underbrace{\left(-i\hbar \frac{\partial}{\partial x}\right)}_{\hat{p}} \Psi(x,t)\, dx$

$$\langle \hat{x}^2 \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t)\, \underbrace{x^2}_{\hat{x}^2}\, \Psi(x,t)\, dx, \quad \langle \hat{p}^2 \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t) \underbrace{\left(-i\hbar \frac{\partial}{\partial x}\right)^2}_{\hat{p}^2} \Psi(x,t)\, dx$$

uncertainty (variance) $\Delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2}$, $\Delta p = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2}$

Example 5: Harmonic oscillator:

$$V(x) = \frac{\hbar^2}{2ma^4} \cdot x^2$$

$$\Psi(x,t) = \psi(x) e^{-\frac{iEt}{\hbar}}$$

$$= N e^{-x^2/2a^2} e^{-\frac{iEt}{\hbar}}$$

is a stationary solution to the S.E.

What is E? N? $\langle \hat{x} \rangle$? $\langle \hat{p} \rangle$? Δx? Δp?

Solution:

The spatial part of the stationary solution satisfies the TISE:

$$\hat{H}\psi(x) = E\psi(x)$$

$$\frac{\partial \psi(x)}{\partial x} = \frac{\partial}{\partial x}\left(N e^{-x^2/2a^2}\right) = N \cdot \left(\frac{-x}{a^2}\right) e^{-x^2/2a^2} = -\frac{x}{a^2}\psi(x)$$

$$\frac{\partial^2 \psi(x)}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}\psi(x)\right) = \frac{\partial}{\partial x}\left[-\frac{x}{a^2}\psi(x)\right]$$

$$= \left[-\frac{1}{a^2}\psi(x) - \frac{x}{a^2}\left(-\frac{x}{a^2}\right)\psi(x)\right]$$

$$= \left(-\frac{1}{a^2} + \frac{x^2}{a^4}\right)\psi(x)$$

$$\hat{H}\psi(x) = \left(\frac{\hat{p}^2}{2m} + \hat{V}\right)\psi(x) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{\hbar^2}{2ma^4}\right)\psi(x)$$

$$= \left[-\frac{\hbar^2}{2m}\left(-\frac{1}{a^2} + \frac{x^2}{a^4}\right) + \frac{\hbar^2}{2ma^4}\right]\psi(x)$$

$$= \frac{\hbar^2}{2ma^2}\psi(x)$$

$$= E\,\psi(x)$$

$$\Rightarrow \boxed{E = \frac{\hbar^2}{2ma^2}}$$

$$1 = N^2 \int_{-\infty}^{+\infty} e^{-x^2/2a^2} \cdot e^{-x^2/2a^2}\, dx = \sqrt{\pi a^2}\, N^2 \Rightarrow N = (\pi a^2)^{-\frac{1}{4}}$$

$$\langle \hat{x} \rangle = \int_{-\infty}^{+\infty} \psi^*(x)\, x\, \psi(x)\, dx = \int_{-\infty}^{+\infty} \left[(\pi a^2)^{-\frac{1}{4}} e^{-x^2/2a^2}\right] \cdot x \cdot \left[(\pi a^2)^{-\frac{1}{4}} e^{-x^2/2a^2}\right] dx$$

$$= 0$$

$$\langle \hat{p} \rangle = \int_{-\infty}^{+\infty} \psi^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x)\, dx = \int_{-\infty}^{+\infty} \left[(\pi a^2)^{-\frac{1}{4}} e^{-x^2/2a^2}\right]\left[-i\hbar\frac{\partial}{\partial x}\right]\left[(\pi a^2)^{-\frac{1}{4}} e^{-x^2/2a^2}\right] \cdot dx$$

$$= 0$$

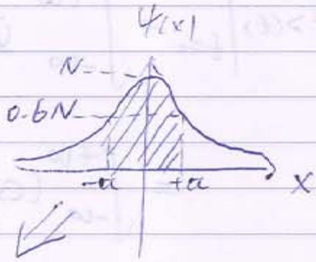
Similarly compute

$\langle \hat{x}^2 \rangle$ and $\langle \hat{p}^2 \rangle$,

$$\Delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2} = \sqrt{\langle x^2 \rangle} = a/\sqrt{2}$$

$$\Delta p = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2} = \sqrt{\langle \hat{p}^2 \rangle} = \hbar/\sqrt{2}a$$

Rough estimation of Δp:



Quite close to the above exact solutions!

$$\begin{cases} \Delta x \approx a \\ \downarrow \text{ Heisenberg uncertainty principle} \\ \Delta p \geq \dfrac{\hbar}{2a} \end{cases}$$

Example 6. Interference (particle in a box)

$$\psi_2(x) = \sqrt{\frac{2}{L}}\sin\frac{2\pi x}{L}, \quad \psi_3(x) = \sqrt{\frac{2}{L}}\sin\frac{3\pi x}{L}$$

$$\Psi(x,t)\Big|_{t=0} = \frac{1}{\sqrt{2}}\psi_2(x) + \frac{1}{\sqrt{2}}\psi_3(x)$$

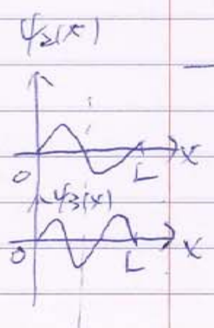
What is $\langle\hat{x}\rangle$ at $t=0$?

Solution: denote $\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}$ by C_2 and C_3:

$$\langle\hat{x}\rangle(t)\Big|_{t=0} = \int_{-\infty}^{+\infty} \Psi^*(x,0) \times \Psi(x,0)\,dx$$

$$= \int_{-\infty}^{+\infty} (C_2^*\psi_2 + C_3^*\psi_3) \times (C_2\psi_2 + C_3\psi_3)\,dx$$

$$= |C_2|^2 \int_{-\infty}^{+\infty} \psi_2(x) \times \psi_2(x)\,dx + |C_3|^2 \int_{-\infty}^{+\infty} \psi_3(x) \cdot x\,\psi_3(x)\,dx + \left[C_2^*C_3\int_{-\infty}^{+\infty} x\,\psi_2(x)\psi_3(x)\,dx + C_2C_3^*\int_{-\infty}^{+\infty} x\,\psi_2(x)\psi_3(x)\,dx\right]$$



$$\int_{-\infty}^{+\infty} \psi_2(x) \times \psi_2(x)\,dx = \langle\hat{x}\rangle_{\text{state }2} = \frac{L}{2} \text{ according to symmetry.}$$

$$\int_{-\infty}^{+\infty} \psi_3(x) \times \psi_3(x)\,dx = \langle\hat{x}\rangle_{\text{state }3} = \frac{L}{2} \text{ according to symmetry.}$$

$|C_2|^2 + |C_3|^2 \equiv 1$: normalization condition

So the non-trivial part is the $\boxed{\text{interference terms}}$.

~~cross products~~

Interference terms:

$$C_2^* C_3 \int_{-\infty}^{+\infty} x \psi_2(x) \psi_3(x) dx \xleftrightarrow{\text{complex conjugate}} C_2 C_3^* \int_{-\infty}^{+\infty} x \psi_2(x) \psi_3(x) dx .$$

$$\int_{-\infty}^{+\infty} x \psi_2(x) \psi_3(x) dx$$

$$= \int_0^L x \psi_2 \psi_3 dx$$

$$= \int_0^L x \cdot \left(\sqrt{\tfrac{2}{L}} \sin \tfrac{2\pi x}{L}\right)\left(\sqrt{\tfrac{2}{L}} \sin \tfrac{3\pi x}{L}\right) dx$$

$$= \left(\sqrt{\tfrac{2}{L}}\right)^2 \int_0^L x \cdot \left(-\tfrac{1}{2}\right)\left(\cos \tfrac{5\pi x}{L} - \cos \tfrac{\pi x}{L} \right) dx$$

$$= \left(\sqrt{\tfrac{2}{L}}\right)^2 \left(-\tfrac{1}{2}\right) \left[\int_0^L x \cos \tfrac{5\pi x}{L} dx - \int_0^L x \cos \tfrac{\pi x}{L} dx \right]$$

$$\downarrow$$

$$\left(\tfrac{5\pi}{L}\right)^{-1} \int_0^L x \, d \sin \tfrac{5\pi x}{L}$$

Integrate by part $\downarrow$

$$\left(\tfrac{5\pi}{L}\right)^{-1} \left[x \sin \tfrac{5\pi x}{L} \Big|_0^L - \int_0^L \sin \tfrac{5\pi x}{L} dx \right]$$

$$\downarrow$$

$$\left(\tfrac{5\pi}{L}\right)^{-1} \left[0 - \left(\tfrac{5\pi}{L}\right)^{-1} (-) \cos \tfrac{5\pi x}{L} \Big|_0^L \right]$$

$$\downarrow$$

$$\left(\tfrac{5\pi}{L}\right)^{-2} (-2) \xrightarrow[\text{replace 5 by 1}]{} \left(\tfrac{1\pi}{L}\right)^{-2} (-2)$$

$$= \left(\sqrt{\tfrac{2}{L}}\right)^2 \left(-\tfrac{1}{2}\right) \left[\frac{L^2}{25\pi^2} - \frac{L^2}{\pi^2} \right] (-2)$$

$$= \frac{2}{L} \cdot \frac{-24 L^2}{25\pi^2}$$

$$= \frac{-48 L^2}{25\pi^2}$$

Interference terms:

$$C_2^* C_3 \int_{-\infty}^{+\infty} x \psi_2 \psi_3 \, dx \; + \; \text{complex conjugate}$$

$$= C_2^* C_3 \cdot \left[-\frac{48}{25\pi^2} L \right] + \text{c.c.}$$

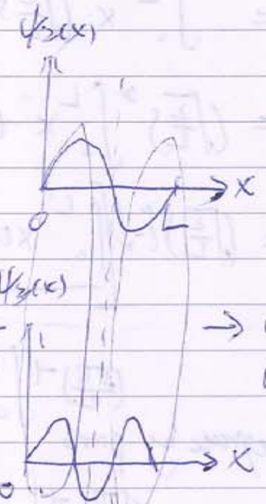
$$= \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} \cdot \left[-\frac{48}{25\pi^2} \cdot L \right] + \text{c.c.}$$

$$= -\frac{48}{25\pi^2} \cdot L$$

$$\Rightarrow \langle x \rangle_{t=0} = \frac{L}{2} + \left(-\frac{48}{25\pi^2} \right) L$$

$$\approx \frac{L}{2} - \frac{1}{5} L$$

$$< \frac{L}{2}$$



constructive interference

destructive interference

consistent with the exact solution.

It should be more likely to find the particle in the LEFT half of the box, intuitively speaking.